How to measure the bandstructures of insulators and semiconductors

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Wide band-gap two-dimensional (2D) materials exhibit interesting optical properties such as highly tunable photoluminescence across the visible range [1] and room temperature deep ultraviolet emission [2]. The underlying electronic excitation spectrum that defines such properties has not been studied in detail by direct energy- and momentum-resolving probes such as angle-resolved photoemission (ARPES). This method can be challenging to apply to highly gapped materials due to photo-induced charging. We circumvent this issue here using micro-focused ARPES (microARPES) at the MAESTRO facility at the Advanced Light Source.

We focus on layered III-VI semiconductors based on gallium chalcogenides such as GaSe, which consists of van der Waals stacked Se-Ga-Ga-Se tetralayers as shown in Fig. 1(a). In these materials, the optical and electronic band gaps can be efficiently engineered by controlling the thickness of the materials or by alloying with different amounts of sulphur and selenium. We investigate the valence band dispersion in cleaved GaSe crystals and track the dispersion changes for different alloy compositions in GaS_xSe_{1-x} (see Fig. 1(b)-(c)) as well as the effect of intercalating alkali metals between the GaSe tetralayers. The changes in the quasiparticle band structure are consistent with the optical transitions measured by photoluminescence. The measured electronic properties of the Ga chalcogenides are compared with microARPES experiments on other important 2D wide-gap systems such as hexagonal boron-nitride (hBN), and the implications for designing new types of van der Waals heterostructures are discussed.

References:
[1] C. S. Jung, F. Shojaei *et al.*, ACS Nano **9**, 9585 (2015).
[2] T. Tran, K. Bray *et al.*, Nature Nanotechnology **11**, 37 (2016).

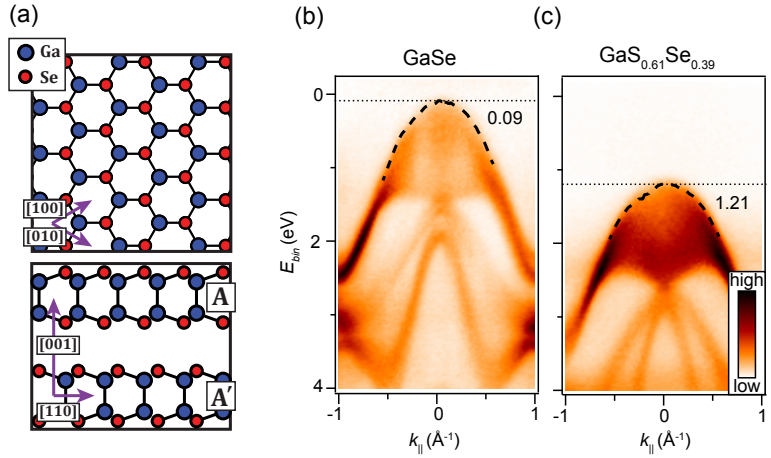

Figure 1: (a) Crystal structure of GaSe in the AA' stacking sequence. (b)-(c) microARPES measurements of the upper valence band dispersion of (b) GaSe and (c) GaS_xSe_{1-x} for x = 0.61. The valence band offset is given in units of eV.